

Spin Dependent Near-Edge X-ray Absorption Measurements of $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$: The Role of Jahn-Teller Distortions in Determining the Spin Polarization of the 4p-Band

Q. Qian, T.A. Tyson (New Jersey Institute of Tech.), C.-C. Kao (NSLS), and M. Croft (Rutgers U.)

Abstract No. qian6703

Beamline(s): X21

Introduction: Spin polarized x-ray absorption spectroscopy (SPXAS) was first performed by Hamalainen *et al*¹ on MnO and MnF_2 . Although the signal to noise was poor, the approach opened the way for 3d elements spin polarized x-ray absorption spectroscopy. Groot *et al*² measured and calculated the MnP SPXAS, producing a detailed interpretation of the emission spectra. We have applied this approach to CMR materials to ascertain the doping and temperature dependence of the spin density of states. The results can be compared with spin dependent density of state calculations including bandstructure calculations.

Methods and Materials: Samples of $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$ series were synthesized and characterized as described in Ref. [3]. Samples were prepared by finely grinding the materials and packing them onto adhesive tape. The Mn SPXAS measurements were performed at X21A. Five spherically bent Si (220) analyzer crystals were used in a Rowland circle⁴ to resolve emitted photons energy. The resolution of this analyzer was 0.7eV. A solid state Biclon fluorescence detector was used to measure the fluorescence radiation. The method of SPXAS measurement is based on energy resolving the K_β emission spectrum which can separate different Mn 1s spin states due to their different emission energies.¹ Temperature dependent measurements were performed for $x=0$, 0.3, 0.5, 0.7 and 1.0. These were compared with room temperature measurements on standard Mn oxides and MnF_2 .

Results:

These spectra give direct information on the Mn partial density of states. We found that for the whole x range a large spin-up spin down splitting exists. The largest splittings 1.2eV is found $x=0.3$. These 4p spin splittings in the main edge are theoretically related to the exchange splitting dependence and Jahn-Teller distortions. Comparisons with standard Mn oxides of known spin and valence are made. We have also studied the temperature dependence of the spin polarized near edge spectra for $x=0$, 0.3, 0.5, 0.7 and 1.0. Large difference in temperature dependence at the pre-edge were found, which are relative to 4p and neighbor 3d hybridization and local distortion. The direct average of the polarized spectra yield curves of similar shape to standard transmission XANES spectra except that spin polarized measurements have higher resolutions (particularly in the near edge region). Work is in progress to model the spectra and extract the spin-polarized density of states.

Acknowledgments: Data acquisition was performed at Brookhaven National Laboratory's National Synchrotron Light Source. The x-ray measurements were supported by Department of Energy, Office of Basic Energy Sciences Grant DE-FG02-97ER45665.

References:¹ K. Hamalainen, C-C. Kao, J. B. Hastings, D. P. Siddons, L. E. Berman, V. Stojanoff, S. P. Cramer, Phys. Rev. B **46**, 14274 (1992).² F. deGroot, S. Pizzini, A. Fontaine, K. Hamalainen, C-C. Kao, and J. B. Hastings, Phys. Rev. B **51**, 1045 (1995).³ M. Croft, D. Sills, M. Greenblatt, C. Lee, S.-W. Cheong, K. V. Ramanujachary and D. Tran, Phys. Rev. B **55**, 8726 (1997).⁴ C.-C. Kao, K. Härmäläinen, M. Krisch, D. P. Siddons, T. Oversluizen and J. B. Hastings, Rev. Sci. Instr. **66**, 1699 (1995).

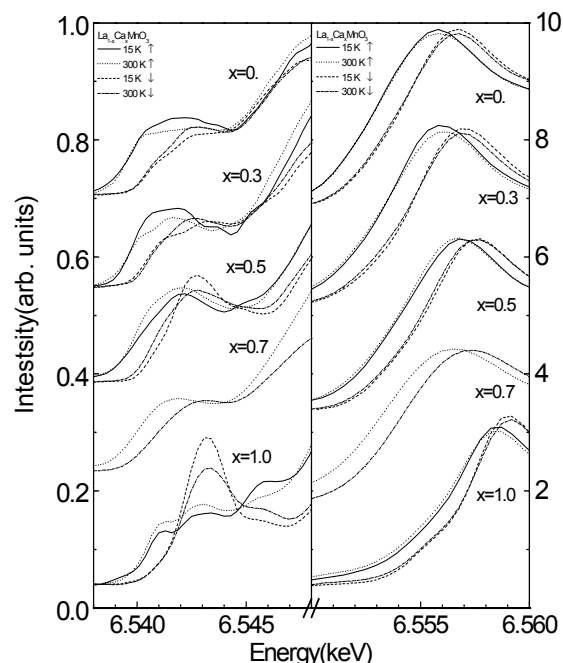


Figure 1. Interlock in special section of spin dependent combined with temperature dependent x-ray K-Edge absorption near edge spectra of $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$ ($x=0, 0.3, 0.5, 0.7, 1.0$). Left panel is in pre-edge region and right panel is in main-edge region. Solid line, 15 K spin up; dotted line, 300 K spin up; dashed line, 15 K spin down; dashed-dotted line, 300 K spin down.